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research note

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Symbol: XTM-RN (U) 97-012

Date: April 22, 1997

SUBJECT: MCNPX — THE LAHET/MCNP CODE MERGER

X-Division Research Note

Executive Summary

The major capabilities of LAHETTM and MCNPTM have now been combined into a prototype version of the merged code MCNPXTM. This report marks the initial release of MCNPX, Version 1.0, and documents the packages from LAHET that have been included in the new code, a new capability for utilizing enhanced cross-section sets, new features of the user interface, some cautions for the user, and the tests that have been performed to date.

I. Introduction

As part of the support for the Accelerator Production of Tritium (APT) program at Los Alamos, groups XTM and T–2 have undertaken the development of a unified code system and associated evaluated data to calculate the cascade of nuclear particles in situations relevant to the APT design process. The resulting software will combine the theoretical models of the LAHET Code System¹ with

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the powerful, general features of the MCNP code² to provide a fully-coupled treatment of the transport problem. Benefits will include the availability of the rich set of variance reduction methods of MCNP, use of MCNP's very general syntax for specifying geometry, sources, and tallies, flexible use of both physical models and evaluated nuclear data, and the provision of a framework for a more consistent treatment of the coupled cascade of nuclear particles. Several preliminary versions³⁻⁷ of this new code have been released. These intermediate versions reworked many aspects of the core MCNP code, to generalize and to prepare for the incorporation of the LAHET modules. MCNPX Version 1.0 is the first release to include a full coupling between the LAHET and MCNP parts of the system.

II. LAHET Modules

All of the LAHET nuclear physics modules are included intact in MCNPX. These include the Bertini⁸ and ISABEL⁹⁻¹⁰ intranuclear cascade (INC) models, the FLUKA¹¹ high-energy generator, the multistage pre-equilibrium exiton model, ¹² the evaporation model, ¹³ the ORNL¹⁴ and RAL¹⁵ (Rutherford Appelton Laboratory) models for fission induced by high-energy interactions, the Fermi breakup model, ¹⁶ the nucleon elastic scattering model, ¹⁷ and the gamma production (PHT) models. The particle decay features of LAHET are also included in their entirety. Transport cross sections, where not determined by MCNPX library methods, are defined as in LAHET. The LAHET data files BERTIN and PHTLIB are now accessed by MCNPX to provide the necessary data for the included LAHET modules. Table 1 shows the list of particles capable of being transported with this release of MCNPX. The table is a subset of the corresponding table in Ref. 4, representing only the currently implemented particles in the MCNP and LAHET parts of the combined code. Both particles and antiparticles are listed, since they are treated differently by the code.

III. Charged-Particle Processes

The mean collisional energy-loss rates for charged particles other than electrons are calculated using an approximate treatment ¹⁸ based on the corresponding calculation for electrons. This treatment will be replaced with the methods from LAHET in the next version of MCNPX. The energy-loss straggling is sampled using a prototype implementation ¹⁹ of the Vavilov theory. This module will also be updated or replaced in a future version of the code.

IV. Evaluated Particle-Production Data

An important requirement of the code and data development for APT is to develop the necessary tools to model transport of coupled neutral- and charged-particles below 150 MeV based on nuclear-data evaluations. This release of MCNPX partially meets that requirement. The physics capabilities of MCNP have been upgraded²⁰ to include the production of secondary charged particles from neutron collisions using data contained on expanded continuous-energy neutron cross-section tables.

Table 1: Transportable Particles in MCNPX, Version 1.0

IPT	JAN	Name of Particle	Symbol	Mass in MeV	Default Energy Cutoff
1	1	neutron	n	939.58	0.0
1	-1	anti-neutron	n	939.58	0.0
2	0	photon	p	0.0	0.001
3	_	electron	e	0.511008	0.001
3	_	positron	e	0.511008	0.001
4	1	muon		105.658389	0.11261
4	-1	anti-muon		105.658389	0.11261
6	1	neutrino_e	u	0.0	0.0
6	-1	anti-neutrino_e	u	0.0	0.0
9	1	proton	h	938.27231	1.0
9	-1	anti-proton	h	938.27231	1.0
20	1	pi_+	\	139.56995	0.14875
20	-1	anti-pi_+	\	139.56995	0.14875
21	0	pi_0	z	134.9764	0.0
22	1	k_+	k	493.677	0.52614
22	-1	anti-k_+	k	493.677	0.52614
23	1	k_0_short	%	497.672	0.000001
24	1	k_0_long	^	497.672	0.000001
31	1	deuteron	d	1875.627	1.0
32	1	triton	t	2808.951	1.0
33	1	helium_3	S	2808.421	1.0
34	1	alpha	a	3727.418	1.0

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An expanded format for MCNP continuous-energy data tables, to permit an arbitrary number of secondary-particle species, was defined in Refs. 23 and 24. An auxiliary processing code²⁵⁻²⁷ called ADDCP has been written to create MCNP data tables in this expanded format. The current neutron data library resulting from these efforts contains cross-section tables for 15 isotopes and is described in the forthcoming Ref. 28.

In order to use these new evaluations and the corresponding data tables, the routines in MCNP for reading cross sections and for sampling secondary particles have been expanded. The modifications have been managed so that the methods applicable to neutron-induced charged-particle production are very similar to the existing methods for neutron-induced photon production. As in the existing neutron algorithm, the code performs a significant amount of pre-transport data manipulation. In particular, the list of active particle types, determined on the MODE card, is used to expunge unneeded data for the problem. Neutron heating numbers are also modified based on the charged particles to be transported.

At every neutron collision, the possibility exists to produce secondary charged particles. All data used in the sampling process are specific to the collision isotope and are evaluated at the incident neutron energy. The expected weight of a particular charged particle i is

$$WGT \cdot \sigma_{cp, i}(E) / \sigma_{tot}(E)$$
,

where WGT is the weight of the incident neutron, $\sigma_{cp,\,i}$ is the total particle-production cross section, σ_{tot} is the total neutron-interaction cross section, and E is the incident neutron energy. The number of charged particles produced is an integer (possibly 0) determined by analog sampling. If the code determines that a charged particle will be produced, it then samples the reaction responsible for that particle. There is no correlation between the reactions sampled as being responsible for the various secondary particles that may be produced as a result of a single neutron collision.

MCNPX supports several ENDF6 representations of scattered energy-angle distributions. Specifically, the following representations for secondary charged particles are allowed: tabular energy distributions, angular distributions via equally-probable cosine bins, Kalbach systematics for correlated energy-angle distributions, discrete two-body scattering, and n-body phase-space energy distributions. In all cases where necessary, kinematics algorithms currently incorporated in MCNP that are specific for neutron-in, neutron-out physics have been generalized to be appropriate for neutrons in and charged particles out. In addition, a general center-of-mass to laboratory conversion technique has been incorporated based on Ref. 29. As is currently the case

for neutron production, all such conversions are based on the assumption of two-body kinematics, which is clearly only an approximation for many of the high-energy neutron reactions represented in APT data evaluations.

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V. User Interface

A great deal of the familiar MCNP user interface either remains unchanged, or is generalized in a very obvious way. For example, the MODE card now accepts any of the particle designators in the table of transportable particles. Thus for a transport problem involving neutrons, protons, deuterons, tritons, ³He's, and alphas, but with no other particles of interest, one would specify

to identify the active particles for the problem. In the absence of a particle type specified on the SDEF card, MCNPX follows the usual rule: the source is the active particle type with the lowest value of IPT. To specify a different source particle on the SDEF card, one uses the numerical value of IPT for the desired particle. Thus a proton source may be requested by

An enhancement of this syntax allows the definition of antiparticle sources. Thus the card

specifies an antiproton source. The only exception to this enhancement is that positron sources have not yet been implemented.

As with neutrons and electrons (but not photons), the first entry on the PHYS:pl card specifies a maximum energy relevant to that particle type. If the user fails to give a maximum energy for each particle active in the problem, the code attempts to select a reasonable value, which will be the largest maximum energy given on PHYS cards for active particles. If no maxima are specified anywhere, the code will use 100 MeV. If particles are ignored during transport because of excessive energy, a warning is issued, and a diagnostic table is printed. The user should especially pay attention to the maximum energies in the case of source particle types that can decay or annihilate. Electrons are a special case in that their maximum energy is not allowed to exceed 1 GeV, which is the highest energy for which electron tables are available at the present time.

For all particle types, the second entry on the CUT:pl card determines the energy cutoff for that particle type. MCNPX contains an array of minimum allowed energy cutoffs, and a second array (currently identical) of default energy cutoffs for each particle type. These values are determined by considerations of the validity of the various theories as applied to the different particles, including consideration of the particle mass. If the user does not enter an energy cutoff for a given particle, then the default value is used.

MCNPX follows neutrons using either the physical models of LAHET, or the evaluated data in nuclear data tables. In the current version, this choice is made for all materials in the problem at a single energy. If the user does not specify this energy, then it is 20 MeV. However, the user can select a different "cross-over" energy below which the code will rely on tabular data by giving a value as the third entry on the PHYS:N card. This is an important feature if one is using the new 150-MeV data tables, for example. A future version of MCNPX will automatically make the distinction between tabular data and physical models in an isotope- and energy-dependent way. However, it should be emphasized that this release of the code expects *all* isotopes in the problem to have neutron data tables below the "cross-over" energy.

Tallies may be requested in the obvious way. For example, a proton surface current tally on surfaces 10 and 11 with two energy bins (and a total energy bin) would result from

f1:h 10 11 e1 100. 1000.

At present, only tally types 1, 2, and 4 are expected to work for the newly-supported particle types with IPT > 3.

Other particle-dependent input cards, including cell importances, IMP:pl, cell-dependent energy cutoffs, ELPT:pl, and energy splitting, ESPLT:pl, will probably work, but have not been tested. Some particle-dependent options, including exponential transform, forced collisions, weight windows, perturbations, DXTRAN, and detectors, have not yet been implemented, and should not be used.

A temporary feature is that a nonzero sixth entry on the DBCN card allows the banking, but prevents the further transport of particles with IPT > 3. This feature in intended only for debugging the secondary particle production algorithms, and will be removed in a future version of the code.

Finally, the control of the physics options in the LAHET part of the code requires additional input syntax, as described in the next section.

VI. Four New Input Cards

Four new MCNPX input records have been defined to allow user control of the physics options. These cards are designated LCA, LCB, LEA, and LEB. A brief summary of these cards follows. More details are given in the various references. All of the input values have defaults, which will be taken in the absence of the cards, or with the use of the MCNP-style "J" input option.

LCA IELAS IPREQ IEXISA ICHOIC JCOUL NEXITE NPIDK NOACT

IELAS:

0 -- no nucleon elastic scattering;

1 -- elastic scattering for neutrons only;

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2 -- elastic scattering for neutrons and protons (default). For a description, see Ref. 17.

IPREQ:

- 0 -- no pre-equilibrium model will be used (default);
- 1 -- use pre-equilibrium model¹² after intranuclear cascade;
- 2 -- use IPREQ = 1 and IPREQ = 3 randomly, with an energy-dependent probability that goes to IPREQ = 3 at low incident energies and to IPREQ = 1 at high incident energies;
- 3 -- use pre-equilibrium model instead of the intranuclear cascade.

Options IPREQ = 2 and IPREQ = 3 apply only when using the Bertini intranuclear cascade model (IEXISA = 0); when using the ISABEL model, these options default to IPREQ = 1.

IEXISA:

- 0 -- do not use ISABEL intranuclear cascade model for any particles;
- 1 -- use Bertini model for nucleons and pions, with ISABEL model for other particle types (default);
- 2 -- use ISABEL model for all incident particle types.

The ISABEL intranuclear cascade model requires a much greater execution time. In addition, incident energies should be less than 1 GeV, or 1 GeV per nucleon for composite particles (although it may execute at higher energies). See Ref. 9, 10, and 30.

ICHOIC: Controls options for the ISABEL INC model. The default is 23 (i.e., 0023). For usage, see Ref. 1.

JCOUL:

- 1 -- use Coulomb barrier on incident charged particle interactions (default);
- 0 -- no Coulomb barrier for incident charged particles.

The methodology is described in Ref. 31.

NEXITE:

- 1 -- subtract nuclear recoil energy to obtain nuclear excitation energy (default);
- 0 -- do not subtract nuclear recoil energy.

See Ref. 32 for a discussion.

NPIDK:

- 1 -- force π^- to terminate by decay at the pion cutoff energy;
- 0 -- force π^- to interact by nuclear capture (intranuclear cascade) when cutoff is reached (default).

The capture probability for any isotope in a material is proportional to the product of the number fraction and the charge of the isotope. However, capture on ¹H leads to decay rather than interaction.

NOACT:

- 1 -- do not turn off nonelastic reactions (default);
- 0 -- turn off all nonelastic reactions.

The use of the NOACT option is intended as a diagnostic tool, allowing other processes to be more easily observed.

LCB FLENB₁ FLENB₂ FLENB₃ FLENB₄ FLENB₅ FLENB₆ CTOFE FLIMO

FLENB₁ FLENB₂: For nucleons, the Bertini INC will be used below FLENB₁ whereas above FLENB₂ the FLUKA high-energy generator¹¹ will be used. The probability for selecting the interaction model is interpolated linearly with incident energy between these limits. The defaults are 2500 MeV and 5000 MeV, respectively.

If FLENB1 = FLENB2 then the transition between models is made at that unique energy; the ability to "phase in" the transition between models over an energy range is largely for "cosmetic" purposes. The lower limit (incident momentum) for the FLU-KA model is 500 MeV/c. For nucleons, the Bertini model switches to a scaling procedure above 3.495 GeV, wherein results are scaled from an interaction at 3.495 GeV. Although both models will execute to arbitrarily high energies, a plausible upper limit for the Bertini scaling law is 10 GeV.

FLENB₃ FLENB₄: For pions, these input parameters act as the above. The defaults are 2500 MeV and 5000 MeV, respectively. Note that for pions, the Bertini model switches to the scaling law method above 2.495 GeV.

FLENB₅ FLENB₆: These input parameters act like the pairs described above, but define the transition to the ISABEL INC below FLENB₅ to one of the higher energy models above FLENB₆ as appropriate for particle type and energy range. The defaults are 500 MeV and 1000 MeV, respectively.

For IEXISA = 2, it applies to all particle types;

for IEXISA = 1, it applies to all except nucleons and pions;

for IEXISA = 0, it is immaterial.

Consider the following example:

lcb 3000 3000 2000 2000 1000 1000

For IEXISA = 1, the default, nucleons would switch to the Bertini model from the FLUKA model below 3 GeV and pions would switch below 2 GeV. Kaons and antinucleons would switch to the ISABEL model from the FLUKA model below 1 GeV. (Ions use only the ISABEL model and muons have no nuclear interactions in LAHET). For IEXISA = 2, nucleons and pions would also switch to the ISABEL model below 1 GeV. Note that the nominal upper energy limit for the ISABEL model is about 1 GeV/nucleon; it may actually execute at higher energies without "crashing," but with diminished validity.

CTOFE: Controls the cutoff energy for emitting particles in the Bertini model. The default is -1. For usage, see Ref. 1.

FLIM0: Controls mass-energy balancing in the cascade stage.

The default is -1. For usage, see Ref. 1.

LEA IPHT ICC NOBALC NOBALE IFBRK ILVDEN IEVAP NOFIS

IPHT:

- 0 -- do not generate photons in the evaporation stage;
- 1 -- generate deexcitation photons (default).

ICC: Defines the level of physics to be applied. Values of 0 through 4 are allowed.

The default is 4. For the definitions of the physics options, see Ref. 1.

NOBALC:

- 0 -- use mass-energy balancing in the cascade stage;
- 1 -- turn off mass-energy balancing in the cascade stage (default).

A forced energy balance may distort the intent of any intranuclear cascade model. Energy balancing for the intranuclear cascade is controlled by input parameter FLIM0.

NOBALE:

- 0 -- use mass-energy balancing in the evaporation stage (default);
- 1 -- turn off mass-energy balancing in the evaporation stage.

IFBRK:

- 1 -- use Fermi breakup model for $A \le 13$ and for $14 \le A \le 20$ with excitation below 44 MeV (default);
- 0 -- use Fermi breakup model only for $A \le 5$.

ILVDEN:

- -1 -- use original HETC level density formulation;
- 0 -- use Gilbert-Cameron-Cook-Ignatyuk level density model¹² (default);
- 1 -- use the Jülich level density parameterization³³ as a function of mass number.

IEVAP:

- 0 -- the RAL evaporation-fission model 15 will be used (default);
- 1 -- the ORNL evaporation-fission model¹⁴ will be used.

The ORNL model allows fission only for isotopes with $Z \ge 91$.

NOFIS:

- 1 -- allow fission (default);
- 0 -- suppress fission.

LEB YZERE BZERE YZERO BZERO

YZERE: The Y0 parameter in the level density formula for $Z \le 70$.

The default is 1.5; zero or negative is an error condition. For target nuclei with $Z \le 70$, the parameters BZERE and YZERE are used to compute level densities; the default values are those used in LAHET before installation of the ORNL fission model. For target nuclei with $Z \ge 71$, the BZERO and YZERO parameters are used to compute level densities for the target nucleus and the fission fragments. Applies only for ILVDEN = -1.

BZERE: The B0 parameter in the level density formula for $Z \le 70$. The default is 8.0; zero or negative is an error condition (see YZERE above). Applies only for ILVDEN = -1.

YZERO: The Y0 parameter in the level density formula for $Z \ge 71$ and all fission fragments. The default is 1.5; zero or negative is an error condition (see YZERE above). Applies only for ILVDEN = -1.

BZERO: The B0 parameter in the level density formula for $Z \ge 71$ and all fission fragments. The default is 14.0 for IEVAP = 0 and is 10.0 for IEVAP = 1; zero or negative is an error condition (see YZERE above). Applies only for ILVDEN = -1.

VII. Caveats and Cautions

This first release of MCNPX does not include a multiple-scattering model for the angular deflection of charged particles other than electrons. This is less significant for APT applications than it might be for other potential applications of the new code. Nevertheless, the implementation of an appropriate scattering model is a high priority for the next release of the code.

The enhanced treatment of tabulated neutron data includes the mechanism to allow the code to take account of the list of active particles in the setting of neutron heating numbers. Thus the groundwork has been laid for a consistent treatment of heating. However, the current 150-MeV neutron data tables do not include the appropriate heating information. Furthermore, the links to heating tallies in the newly-included LAHET modules have not been completed. Therefore, one should not expect type 6 tallies to work properly in this version of MCNPX. Providing this capability is also a high priority for the next release.

The prototype mean-energy-loss model in the present code becomes inaccurate at low energies, and, in fact, can predict negative energy losses at sufficiently low energies for massive charged particles. The user should consult print table(s) 85 to make sure that the energy cutoffs are high enough to avoid this situation. This energy-loss model will also be improved or replaced in forth-coming releases of MCNPX.

The prototype Vavilov straggling model in the present code has been found to have problems in the limit of large step sizes. For other reasons, mentioned in Ref. 19, we want to replace this routine with another model. Therefore, this component is also intended for replacement in later versions of MCNPX.

The user should take care that the maximum energies specified for various particles are high enough to accommodate secondary particles created by annihilation and decay processes. To monitor this, the diagnostic table of particles not banked because of excessive energy is important to watch.

Energy cutoffs that are unnecessarily low can slow the transport calculation down considerably. This is especially true for electrons. The user should take care that energy cutoffs are no lower than needed in a given problem.

Another aspect of calculational speed concerns the substeps taken by charged particles during transport. These substeps are implemented to improve the tracking of angular deflections. Since the current version of MCNPX does not implement angular deflections for charged particles other than electrons, these substeps are actually not needed for the time being. As a temporary expedient, they may be eliminated for all charged particles by setting <code>estep=1</code> on all material cards. This should not be done in problems involving electron transport, since the electrons do have an implemented angular deflection algorithm. In future versions of MCNPX, this problem will be solved by generalizing the substep bookkeeping in a particle-dependent way.

Some of the particle symbols in Table 1 have changed from those used in previous interim versions of MCNPX. The changes were needed to avoid certain characters with special meaning to the text parser of MCNP. These symbols may well change again in future versions, if we devise more convenient ways of parsing the MCNPX input file.

VIII. Testing

As always in MCNP development, the standard set of 29 test problems are an essential part of the software quality assurance procedure. Tests of the current release were performed on machine RHO, where Version 1.0 of MCNPX passes 28 of the 29 test problems, as determined by the MCTL* files. The OUTP* files also agree in 28 out of 29 cases, except for trivial format changes necessary for the code to support the expanded particle set. The exceptional case is problem 17, a multigroup criticality problem. Here the random number sequence and all but two tally bins track the public code. There is reason to believe that the disagreement relates to a subtle problem in the dynamically allocated memory of MCNP. However, the discrepancy remains under investigation.

New test problems have also been created to serve as internal self-consistency checks on the algorithms implemented to create neutron-induced charged particles based on tabular data. It is possible to arrive at the total weight of each secondary charged-particle species produced (per history) by two independent means. The first is through the accounting of particle production by "tabular sampling" that is now displayed automatically in the particle summary tables. The second is by calculating FM tallies using the MT=200 series of total particle-production cross sections calculated by NJOY. These methods should give equivalent, but independent, results for neutron energies above 20 MeV. Results from several such calculations will be documented in Ref. 28. The agreement between the two methods is quite good. These test problems only confirm the algorithms involved in sampling the weight of secondary charged particles; they do

not validate the algorithms used to sample the secondary energy and angular distributions of such particles. Attention to this matter has been provided thus far via hand calculations and code debugging. Additional validation of these algorithms, including calculation of experimental benchmarks, is planned.

Additional test problems have been developed concentrating on the LAHET-based features of MCNPX. These problems have been chosen to test the logic for the handling of the new particle types and the interplay among transport, interaction, and decay. They have been used to observe the tracking changes as code modifications have occurred and to test the setting of defaults within the new code. Incident particles employed in the base test set include protons, neutrons, positive and negative pions, deuterons, antiprotons, and positive muons. The latter case was run as a coupled muon-electron-photon case. Since the incident energy for the base set was 256 MeV in all cases, not all physics modules were executed, notably the high-energy physics options. However, the Bertini and ISABEL intranuclear cascade models, the default evaporation and fission model, the pre-equilibrium model, the gamma deexcitation model, elastic nucleon scattering, and particle decay have been executed successfully. Complete balance has been achieved in the summary tables, including the processes of particle decay and antiparticle annihilation. Two other problems have been devised in both LCS and MCNPX forms which, over time, will lead to direct comparisons. The first is a standard LCS test problem for the neutron spectrum produced from 256-MeV protons on a stopping length ²³⁸U target. The other is a calculation of the flux spectrum for protons at various depths as the particles slow down in thick aluminum. The latter problem is very sensitive to the details of the slowing-down process. The former test problem is relatively insensitive to that feature. A brief examination of Table 2, on the next page, shows that good agreement in the emitted angular neutron current is obtained.

Finally, the INP file for Saturne 800-MeV lead target model was modified to use a proton source and executed with MCNPX for 1000 proton histories (1% of the standard LCS calculations). The calculation executed with no difficulty. The calculated manganese capture rate was about 6 standard deviation away from the most comparable LAHET3.0 calculation. However, the use of a different source distribution, a different slowing-down model, and energy straggling rather than range straggling are likely to play a significant part in explaining the discrepancy.

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LCS Angular Bin **MCNPX** $180.0^{\circ} - 155.0^{\circ}$ 1.78946E-01 (0.0136) 1.81570E-01 (0.0136) $155.0^{\circ} - 145.0^{\circ}$ 1.62713E-01 (0.0140) 1.63831E-01 (0.0140) $145.0^{\circ} - 125.0^{\circ}$ 4.27562E-01 (0.0111) 4.28267E-01 (0.0111) $125.0^{\circ} - 115.0^{\circ}$ 2.43428E-01 (0.0125) 2.48396E-01 (0.0125) $115.0^{\circ} - 62.5^{\circ}$ 1.27044E+00 (0.0091) 1.27182E+00 (0.0093) $62.5^{\circ} - 57.5^{\circ}$ 1.14667E-01 (0.0152) 1.15524E-01 (0.0154) $57.5^{\circ} - 32.5^{\circ}$ 5.08595E-01 (0.0099) 5.07456E-01 (0.0101) $32.5^{\circ} - 27.5^{\circ}$ 8.22157E-02 (0.0171) 8.23298E-02 (0.0172) $27.5^{\circ} - 0.0^{\circ}$ 2.31732E-01 (0.0118) 2.32618E-01 (0.0119) 3.22030E+00 (0.0085) 3.23182E+00 (0.0086) total

Table 2: Energy-Integrated Neutron Current into Angular Bins

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